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Determination of the mechanical properties of corn grains and olive fruits required in DEM simulations.

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Abstract. *Discrete element method (DEM) is a numerical technique widely used for simulating the mechanical behavior of granular materials involved in many food and agricultural industry processes. Additionally, this technique is also a powerful tool to understand many complex phenomena related to the mechanics of granular materials. However, to make use of the potential of this technique it is necessary to develop DEM models capable of representing accurately the reality. For that, among some other questions, it is essential that the values of the microscopic material properties used to define the numerical model are accurately determined.*

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The values of the microscopic material properties used in DEM simulations can be obtained using two possible methods: calibration procedures and direct experimental measurements. Since these properties must be obtained at a particle (microscopic) level, there is still very little information at this regard. Very few procedures have been described in the scientific literature and, in addition, very little accurate information about the values of the material properties is available so far.

The present paper focuses on the determination of the microscopic properties of corn grains and olive fruits used in DEM simulations. For that, the most common procedures used for its direct measurement were initially described. After that, a preliminary material, glass beads, was considered in order to assess the validity of the adopted experimental procedures. Finally, corn grains and olive fruits were tested using the same procedure as for the preliminary material. The following material and interaction properties were considered in the present study: particle density, particle stiffness, particle-wall friction coefficient and particle-particle and particle-wall restitution coefficient. Results obtained are discussed and compared, and some practical recommendations about the use and improvement of these experimental methodologies for the case of irregular particles are presented in this paper.

Keywords. *discrete element method, silo, material properties, corn, olives*

1. Introduction

Discrete element modeling (DEM) is a numerical technique that allows the mechanical static and dynamic behavior of granular materials to be simulated. Developed by Cundall and Strack (1976), it is based on an explicit numerical scheme in which each particle of a system is individually simulated – a requirement when dealing with granular materials. The movement of such granular systems is modeled using laws of motion. Newton's second law of motion is usually used to describe translational movement, and the general rotational dynamics equation to describe rotational movement. The particles are considered to be rigid, but in their movement they are deemed to overlap, producing contact between them. The interaction between the particles is monitored contact-by-contact using a force-displacement law that relates the force involved in the contact between particles with their overlap. The equations that define the movement of and the interaction between particles are very varied (Dziugys and Peters, 2001).

DEM has commonly been used in many industrial areas, such as in the pharmaceutical (Sahni et al., 2010), mining (Whittles et al., 2005) and food industries (Van Zeebroeck et al., 2006) to describe the movement of materials, and in the design of construction, earth-moving (Coetzee et al., 2010) and agricultural machinery (Van Liedekerke et al., 2006). The study of the behavior of granular material in silos and hoppers is another common area where DEM has been used, including the analysis of the pressures exerted by the stored material (Masson and Martínez, 2000), flow patterns (González-Montellano et al., 2011), segregation phenomena (Ketterhagen et al., 2007), the modification of the flow by the inclusion of inserts (Yang and Hsiau, 2001) and the discharge rate (Anad et al., 2008).

The main aim of DEM is to adequately represent a particular real phenomenon. It therefore requires the use of contact models that represent the characteristics of the simulated material as reliably as possible. It also requires the use of values that adequately describe the properties of the material under study. These values can be determined by direct measurements or via calibration procedures. The first method is usually preferable to the second since, in the latter, the adjusted values can be strongly dependent on the numerical code employed in the calibration procedure. However, these properties must be obtained at a particle (microscopic) level and it sometimes makes the direct determination difficult. Until now very few procedures have been described in the scientific literature and, in addition, very little accurate information about the values of the material properties is available.

Because of that, the present paper focuses on the direct determination of the microscopic properties of two agricultural materials: maize and olive fruits. These materials are usually handled in silos and hoppers within the Mediterranean area but very little information is available about their microscopic properties. The existing methods for the direct determination of microscopic properties of particles are very few and are not standardized. In addition there is very little information about them and because of that the direct determination methods considered in this work are firstly described in detail. After that, a well known material (glass beads) was considered as a preliminary step in order to assess the validity of the adopted experimental procedures. Finally, corn grains and olive fruits were tested using the same procedure as for the preliminary material. The following material and interaction properties were considered: particle density (ρ_p), particle stiffness (E_p), particle-wall friction coefficient (μ_w) and particle-particle and particle-wall restitution coefficient (e_p and e_w). Results obtained are discussed and compared, and some practical recommendations about the use and improvement of these experimental methodologies for the case of irregular particles are presented.

2. Direct measurement methods for the determination of microscopic properties of particles.

In this section, the particular methods used for the direct measurement of the microscopic material properties are described. All methods described in this section were used for each of the three materials (glass beads, maize and olive fruits) considered in this work, unless stated otherwise.

Particle density (ρ_p)

Particle density (ρ_p) was estimated using two different methods: METHOD 1 and METHOD 2. In METHOD 1 direct measurements of the particle volume (using an approximation of the real particle shape to a known geometrical shape – see Figure 1 –) and the particle mass (using a precision balance) were taken. In METHOD 2 a technique based on the pycnometer test was used (Figura and Teixeira, 2007). In particular, the total volume of a set of particles was measured by the water displacement method using a measuring cylinder whereas the sample mass was obtained by using a precision balance.

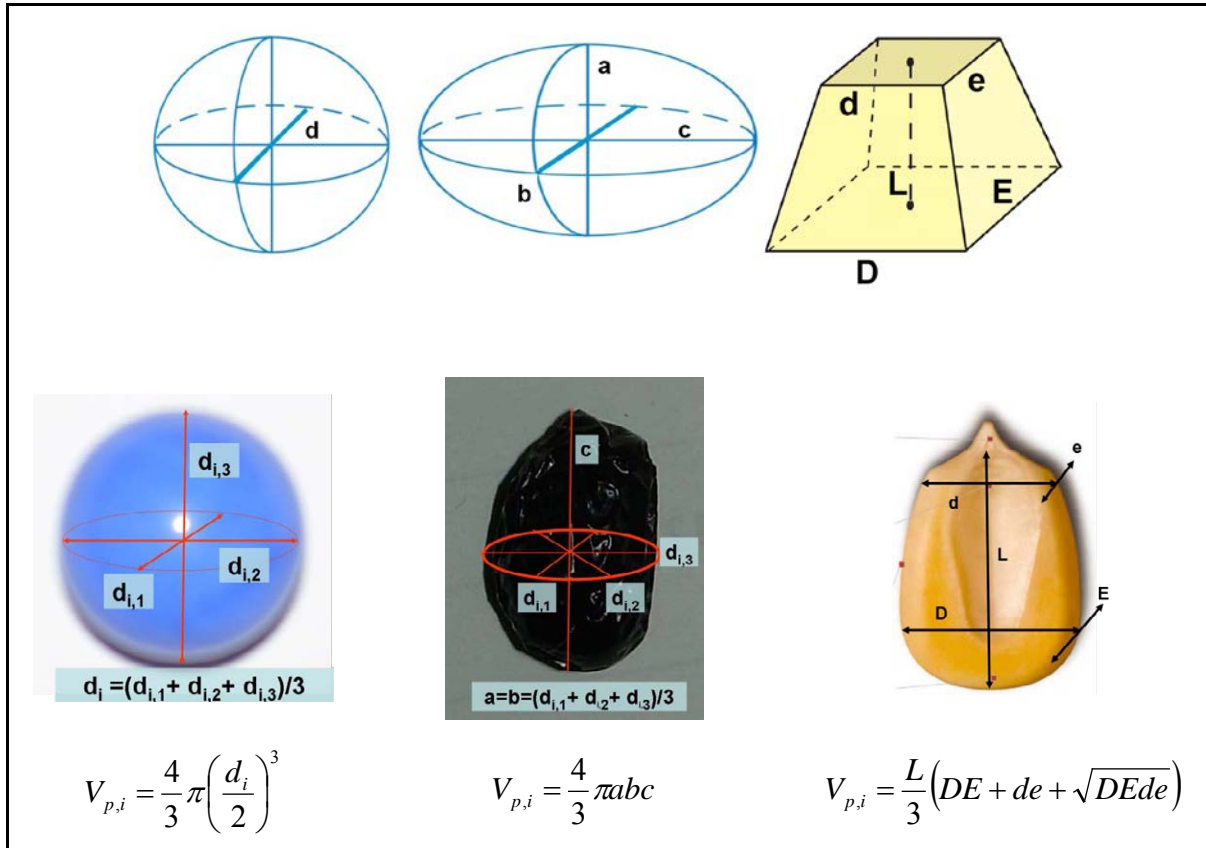


Figure 1. Geometrical shapes used for approximating the real particle shape in METHOD 1

Particle elasticity modulus (E_p)

The value of E_p was only obtained for the case of maize and olive fruits. Glass beads are made of a very well-known material and there exists a big amount of information in the scientific

literature about this value (usually a value of $E_p \approx 40.000$ MPa is adopted). The value of the elasticity modulus for maize and olive fruits was directly measured by using the procedure described in ASAE S368.4 (2006). This procedure is based on a compression test carried out on individual particles using an appropriate compression tool. In the case of maize, a compression test Type D (spherical indenter on a flat surface) was carried out whereas a compression test Type C (spherical indenter on a curved surface) was adopted for olive fruits. In all cases the compression test was carried out using a Texture Analyser TX2 machine (Figure 2). For both materials the spherical indenter used consisted of a steel ball, with a diameter of 4.8 mm and 9.4 mm respectively for the case of maize and olive fruits. A total number of 20 maize particles were analyzed, the compression force being about 30 N applied at a speed of 18 mm/min. In the case of the olive fruits, a total of 30 particles were tested, the compression force being about 0.30 N applied at a speed of 30 mm/min.



Figure 2. Texture Analyser TX2 machine and detail of the compression tool used for maize particles

Particle-wall restitution coefficient (e_w)

The particle-wall restitution coefficient (e_w) was obtained by using a drop test similar to the one described in Gorham and Karaz (2000), Dong and Moys (2006) and Chung (2006). The apparatus used to develop this test was built specifically for this work and consists of the elements shown in Figure 3. In this test one particle of one of the three materials considered (glass beads, corn grains and olives) is released at a certain height H_0 over a flat surface ("the wall") made of two possible materials: methacrylate and steel. This particle impacts on the wall and rebounds, reaching a height H_1 . The whole impact-rebound process is recorded using a high speed camera (Genie H1400-Monochrome) so that this height H_1 can be obtained from the images taken. The coefficient of restitution is obtained in an indirect way as the square root of the ratio H_1/H_0 under the assumption that the rebound is vertical and without rotation.

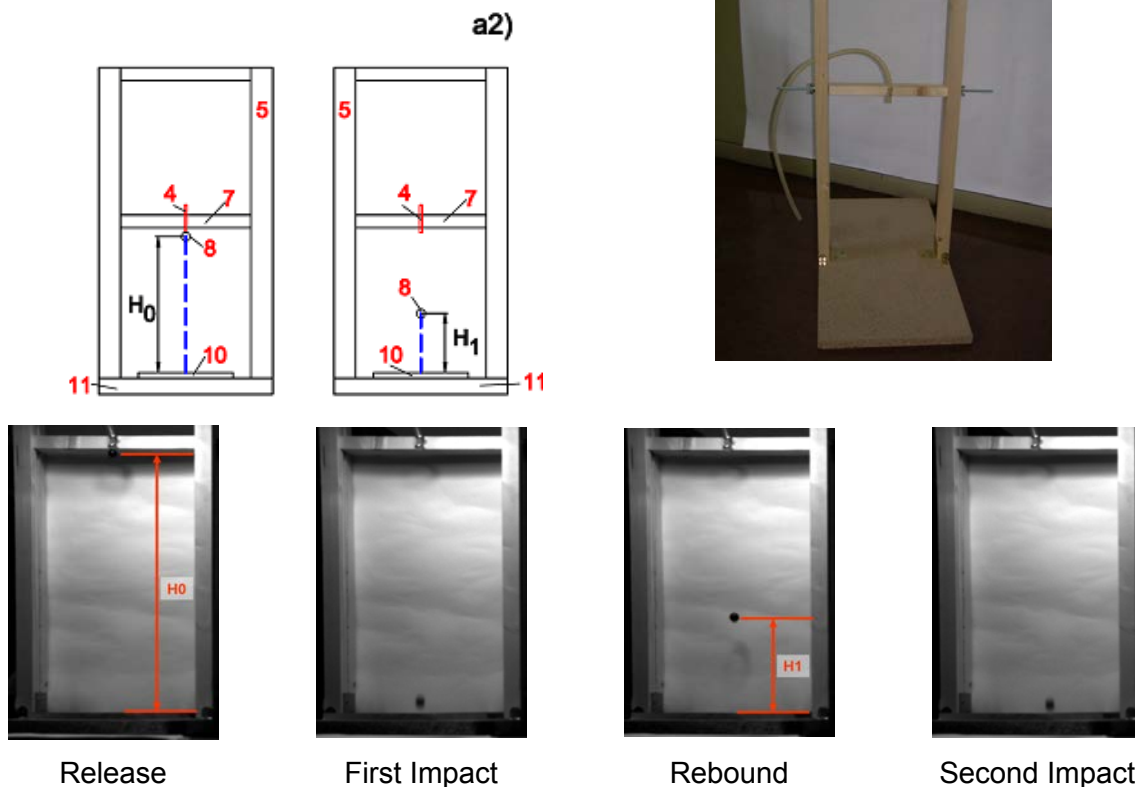
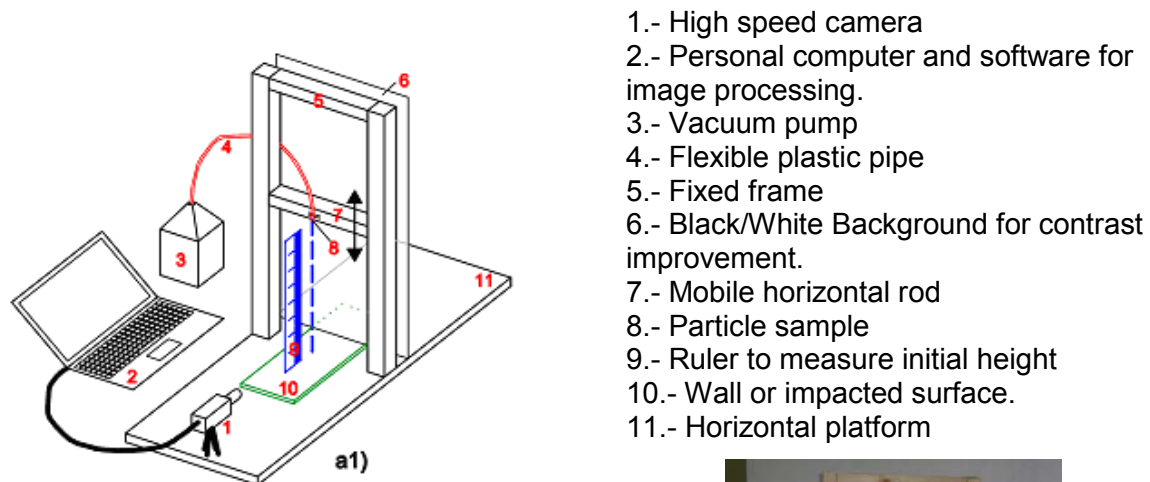
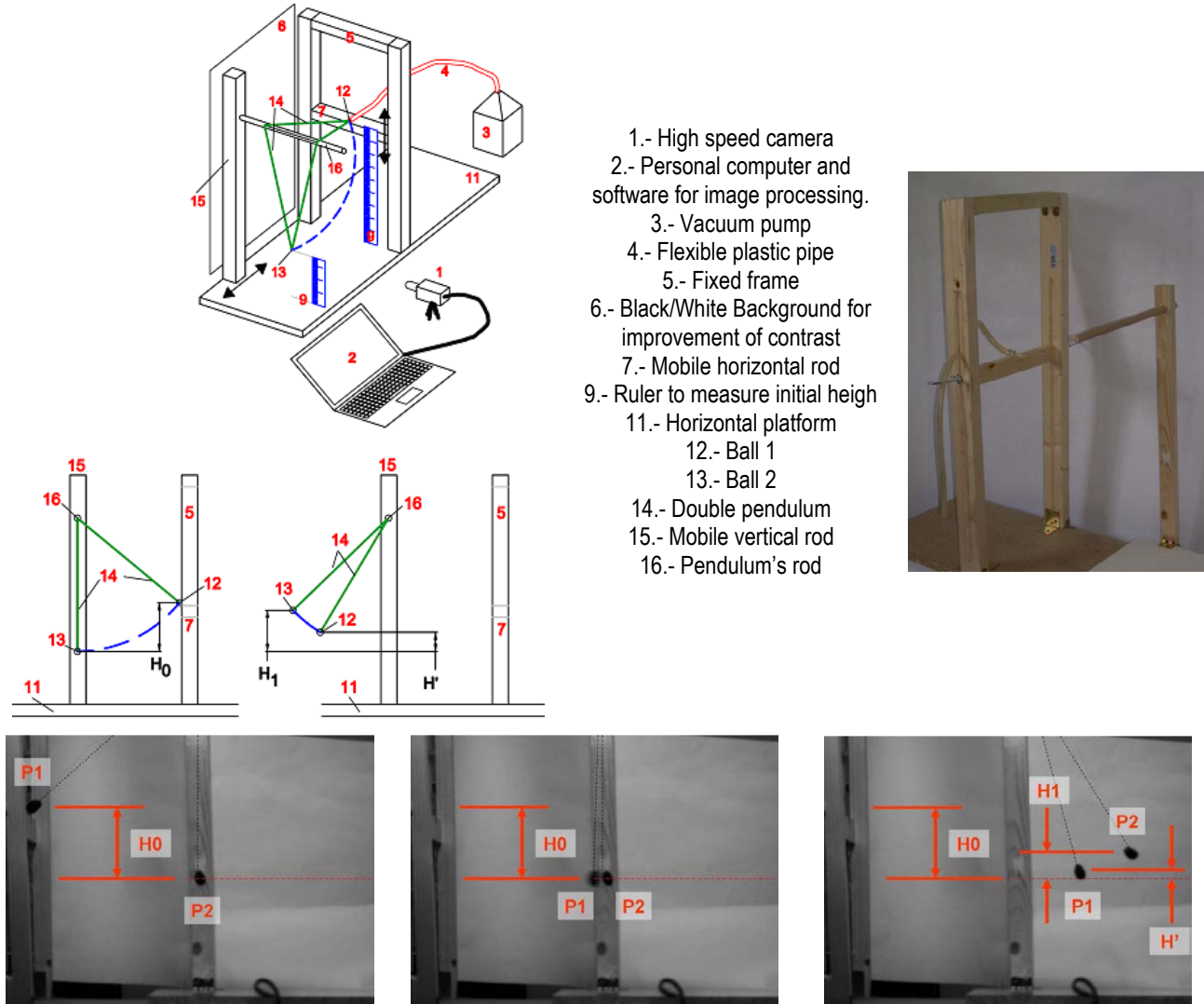


Figure 3. Experimental test for the determination of the particle-wall coefficient of restitution.

Particle-particle restitution coefficient (e_p)

The value of e_p was obtained by using a pendulum test similar to the one described in Wong et al (2009). The apparatus used to develop this test was built specifically for this work and consists of the elements shown in Figure 4. In this test a sample consisting of two individual particles (Ball 1 and Ball 2) of the same material are bonded to two identical pendulums formed with a nylon string. These two pendulums are fixed to a horizontal rod in such a way that both particles are aligned. After that, one of the particles (Ball 1) is laterally moved up to a height H_0

measured from the position of the other particle (Ball 2). Finally Ball 1 is released and collides with Ball 2 reaching, after the impact, heights of H' and H_1 respectively for Ball 1 and Ball 2. In order to be able to measure these characteristic heights, the whole process was recorded using a high speed camera (Genie H 1400-Monochrome) running at 50 fps. The particle-particle restitution coefficient is obtained based on these heights using the expression given in Figure 4.



$$e_p = \frac{\sqrt{H_1} - \sqrt{H'}}{\sqrt{H_0}}$$

Figure 4. Experimental test for the determination of the particle-particle coefficient of restitution.

Particle-wall friction coefficient (μ_w)

The determination of the particle-wall friction coefficient (μ_w) was based on a sliding test similar to the one described in Chung (2006). The apparatus used to develop this test was built specifically for this work and consists of the elements shown in Figure 5. In this test a sample

formed by three particles of the same material placed in a triangular arrangement (sample plate) is fixed to an inclinable base plate. A flat plate (test plate) made of the wall material is placed on top of this sample and the inclination of the base plate is gradually increased until the sliding occurs. At this stage the test stops and the angle of inclination of the base plane is measured in an indirect way to finally obtain the value of μ_w as shown at the end of Figure 5. The materials considered for the sample plate are glass beads, corn grains and olive fruits whereas those used for the test plate are methacrylate and steel.

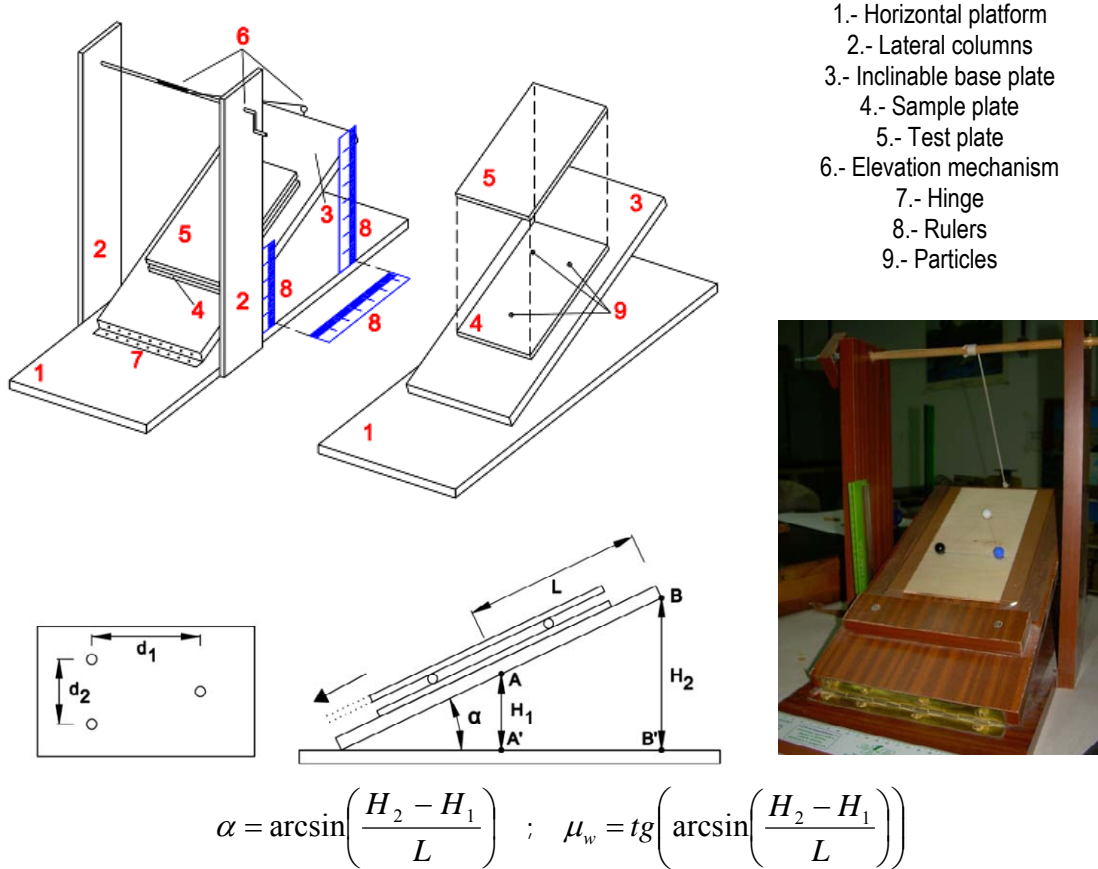


Figure 5. Experimental test for the determination of the particle-wall friction coefficient

3. Results

Particle density (ρ_p)

In Table 1 the results of the particle density determination according to METHOD 1 and METHOD 2 (see Section 2) and for all materials considered are presented. As it can be seen through the values of the coefficient of variation for all materials, METHOD 2 can be considered the most accurate one, since it does not depend on an approximation of the real shape of the particle to calculate their volume. However, differences between methods for the case of glass beads are not very significant since the approximated geometry (sphere) was really close to the real geometry of the particles.

Table 1. Particle density obtained by METHOD 1 and METHOD 2 for all materials considered

	GLASS BEADS		CORN GRAINS		OLIVE FRUITS	
	METHOD 1	METHOD 2	METHOD 1	METHOD 2	METHOD 1	METHOD 2
Number of samples ⁽¹⁾	60	5	60	5	60	5
ρ_p (kg/m ³) ⁽²⁾	2526	2516	879.6	1163	1233	1085
CV (%) ⁽³⁾	2.51	1.24	14.94	0.31	6.21	0.38

(1) In METHOD 1 the number of samples refers to the number of individual particles considered. In METHOD 2 the number of samples refers to the number of sets of particles used.

(2) This is the mean value of the particle density obtained for all samples considered in each method.

(3) This is the coefficient of variation obtained for all samples considered in each method.

In the case of corn grains, the coefficient of variation obtained for METHOD 1 is much bigger than the one obtained for METHOD 2. This information could mean that there is a great dispersion of the values of the particle density for the case of corn grains. However, the mean value for the first method is also rather different than the one obtained in the second. It means that the main problem here is that the geometry used to approximate the real particle shape was not good enough and, in particular, the basic lengths defining that approximated geometry.

As for the olive fruits, the coefficient of variation obtained from METHOD 1 is not much bigger than the one obtained from METHOD 2. However, the mean values obtained for both methods are rather different, what means that the approximated geometry (ellipsoid) was again not good enough. In spite of it, since values of the coefficient of variation from METHOD 1 are not too big, the basic lengths defining the approximated geometry can be considered as valid for the characterization of the olive fruits.

Particle elasticity modulus (E_p)

In Table 2 the resulting mean values of particle elasticity modulus for both materials analyzed (maize and olive fruits) are presented. The values of the coefficient of variation (CV) obtained for both materials are relatively high. It is indicative of the heterogeneity of the material. However, the mean value determined for both materials seems to be different from the values used for other researchers. In the case of maize grains, a mean value of 300 MPa was obtained while in the scientific literature a wider range of values can be found: 1040-2330 MPa (Chung (2006)), 1000 MPa (Tao et al (2010)) or 165-6757 MPa (Shelef and Mohsenin (1967)). Similarly, a mean value of $E = 480$ MPa was calculated for the olive fruits whereas a different value (130-160 MPa) was obtained by Kılıçkan and Güner (2008).

Table 2. Mean values of E_p and coefficient of variations obtained for maize and olive fruits.

CORN GRAINS		OLIVE FRUITS	
E_p MEAN MPa	CV (%)	E_p MEAN MPa	CV (%)
298	24 %	480	30 %

However, these discrepancies do not invalidate the values obtained in the present work due to the following reasons:

- The range of values presented by other authors is quite wide and, particularly in the case of maize, the value obtained in the experiments is included in it.

- Additionally, as concluded in Shelef and Mohsenin (1967), the measured ν value of the elasticity modulus is rather variable depending on many factors: compression test type, size and shape of the compression tool, speed of testing, compression force, particle humidity, particularities of the tested material (such as maturity state, variety.) Therefore it is necessary to establish a common procedure which is considered as valid for all cases.
- In the case of maize the compression test used (spherical indenter on a flat surface) is considered to be more accurate than others where the curvature of the particle needs to be taken into account. This curvature is usually difficult to measure and its value often changes as the specimen is compressed during the test development.

Particle-wall restitution coefficient (e_w)

For the case of the glass beads and for both surface materials, 5 different samples (S1, S2, S3, S4 and S5) have been considered and ten repetitions of the test have been carried out for 5 different initial release heights (H01, H02, H03, H04 and H05). In Figure 6 a graphical representation showing the evolution of e_w with the impact velocity v is included. The value of e_w in Figure 6 represents the mean value calculated for all repetitions and samples considered at a given height H0i. Finally, the impact velocity is obtained as a function of the release height H0i using the expression given in Figure 6.

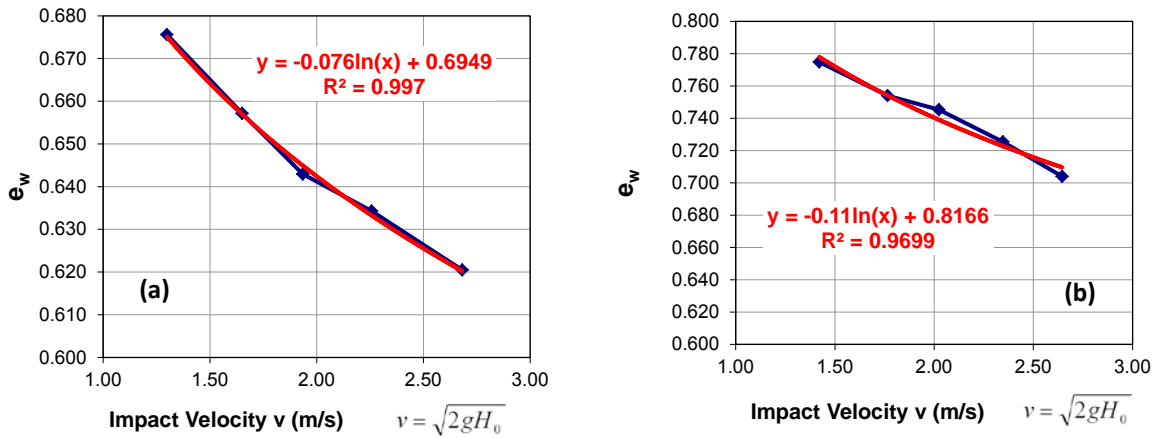


Figure 6. Evolution of e_w with v for the case of glass beads. (a) Methacrylate wall; (b) Steel wall

The value of e_w for glass beads is, for any release height, bigger for the case of a steel wall than for a methacrylate wall. However, in both cases e_w decreases with the impact velocity, as reported in Wong et al (2009). Additionally, the values of the coefficient of variation – CV – are relatively small for both within the ten repetitions of the same sample (≈ 0.5 -1.5 %) and for all samples considered at the same height (≈ 1.5 -2.25 %). It evidences a high repeatability of the test and a noticeable homogeneity of this property for the material considered.

In the case of the corn grains and olive fruits only 10 repetitions for a single sample of each material and for a unique release height were carried out. This is justified by the difficulty of obtaining vertical rebounds without rotation due to the irregularity of the particles of these materials. For the case of maize grains, a mean value of 0.668 (CV = 8.68 %) and 0.748 (CV = 4.40 %) was obtained respectively for a methacrylate wall and a steel wall. Similarly, in the case of olive fruits a mean value of 0.458 (CV = 7.09 %) and 0.454 (CV = 2.33 %) was obtained respectively for a methacrylate wall and a steel wall.

Particle-particle restitution coefficient (e_p)

In the case of glass beads and olive fruits 5 different samples (M1, M2, M3, M4 and M5) for three different release heights H_0 (H_{01} , H_{02} , H_{03}) have been considered and a total number of ten repetitions have been carried out for each combination of sample and release height. For each of these materials, in Figure 7 a graphical representation showing the evolution of the mean particle-particle restitution coefficient with the impact velocity v for all samples is presented. The value of e_w in Figure 7 represents the mean value calculated for all repetitions and samples considered at a given height H_{0i} . Finally, the impact velocity is obtained as a function of the release height H_{0i} using the expression given in Figure 7.

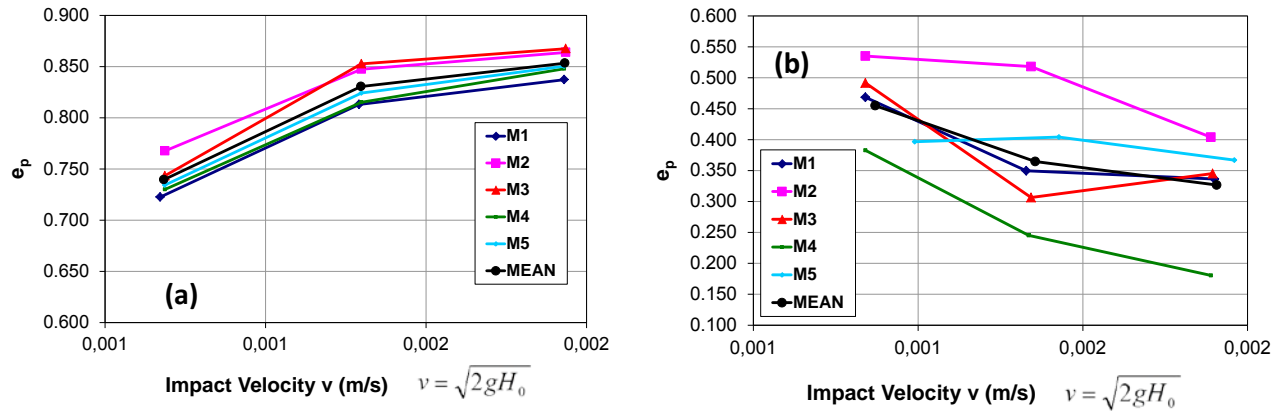


Figure 7. Evolution of e_p with v for the case of glass beads (a) and olive fruits (b).

In the case of the glass beads an increasing trend of e_p with the impact velocity is observed, as previously reported by Wong et al (2009). In addition the values of the coefficient of variation (CV) are relatively small for both within the ten repetitions of the same sample (≈ 0.2 - 0.75 %) and for all samples considered at the same height (≈ 1.3 - 2.2 %). It evidences a high repeatability of the test and a noticeable homogeneity of this property for the material considered.

As for the olive fruits a decreasing trend of e_p with the impact velocity is found. This behavior is thought to be due to the softness of these particles compared to the glass beads. However further investigation is needed to completely understand this observation. Again in this case there is a relatively small value for the coefficient of variation for the ten repetitions carried out for the same sample and release height (≈ 3 - 10 %), which evidences an acceptable test repeatability. However, the coefficients of variation for all samples of a same release height were relatively high (≈ 25 - 30 %), denoting a heterogeneity of the value of e_p .

Finally, in the case of the maize grains, the same number of repetitions and release heights were considered but only three different samples were tested. This is because in this case "clean" impacts were not always achieved and some samples had to be rejected. These "not clean" impacts were caused by the irregularity of the particles together with the small mass of each corn grain, what led to the looseness of the strings forming the pendulums. In Figure 8 a graphical representation showing the evolution of the mean particle-particle restitution coefficient with the impact velocity v is presented. In this case, similarly to the glass beads, the values of e_p increases with the impact velocity, something which is thought to be due to the higher stiffness of these particles compared to the olive fruits. The values of the coefficient of variation are relatively high for both within the ten repetitions of the same sample (≈ 10 - 40 %)

and for all samples considered for the same height ($\approx 15\text{-}38\%$). It evidences a low repeatability of the test (mainly due to the irregularity of the particles and the small mass of each individual grain) as well as a noticeable heterogeneity of this property for the material considered.

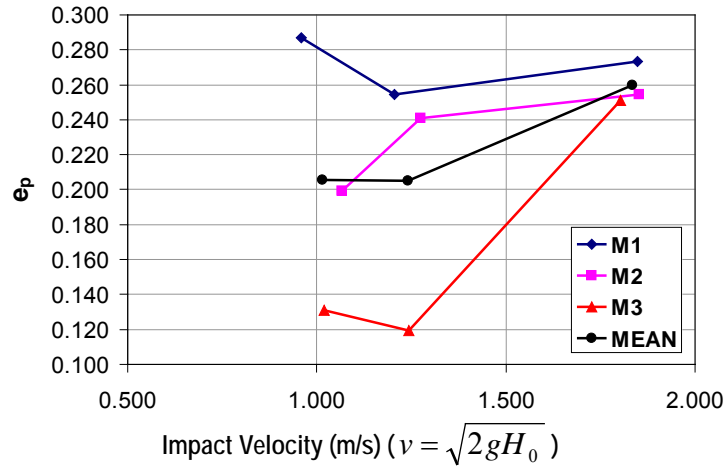


Figure 8. Evolution of e_p with v for the case of maize grains.

Particle-wall friction coefficient (μ_w)

In the case of the particle-wall friction coefficient all materials were tested using the same procedure. For each wall material three different samples (S1, S2 and S3) have been considered and 10 repetitions of the test per sample were carried out. The values of μ_w obtained for each combination are shown in Table 3.

Table 3. Particle-wall friction coefficient for all materials and walls

		GLASS BEADS		CORN GRAINS		OLIVE FRUITS	
		MEAN	CV (%)	MEAN	CV (%)	MEAN	CV (%)
WALL: Methacrylate	S1	0.334	10.65	0.370	9.27	0.523	4.36
	S2	0.284	11.48	0.236	9.85	0.538	9.00
	S3	0.301	6.40	0.378	10.52	0.546	8.69
	TOTAL	0.306	10.82	0.328	21.07	0.533	10.35
WALL: Steel	S1	0.251	8.29	0.218	8.05	0.4	4.89
	S2	0.257	7.89	0.154	8.74	0.345	6.52
	S3	0.245	11.41	0.191	18.86	0.272	7.68
	TOTAL	0.251	9.18	0.188	19.03	0.339	16.85

The values of the coefficient of variation obtained for the case of glass beads and for any type of wall are relatively small both for individual samples and for the whole set of samples. It evidences an adequate repeatability of the test as well as a high degree of homogeneity of this property for this material. However, in the cases of the maize grains or the olive fruits the repeatability is acceptable (not very high values of the coefficient of variation for the same sample) although the homogeneity is not as good as in the case of the glass beads (high values of the coefficient of variation for the whole set of samples). However, these results are normal in real materials as it is the case of corn grains or olive fruits.

Conclusions

The use of DEM models is growing nowadays due to its high capability of properly simulating the mechanical behavior of granular materials. However, the preliminary definition of a DEM model always requires knowing the values of microscopic properties of that material which is being simulated. In this paper the determination of the microscopic material properties for three different materials (glass beads, maize grains and olive fruits) has been carried out. These material properties are: particle density (ρ_p), particle stiffness (E_p), particle-wall friction coefficient (μ_w) and particle-particle and particle-wall restitution coefficient (e_p and e_w). Specific test apparatuses have been designed and built and have been properly described in the paper. In addition to the values of the material properties, results obtained have been discussed and compared, and some practical recommendations about the use and improvement of these experimental methodologies for the case of irregular particles are presented.

In general, the procedures selected to determine the microscopic material properties of the particles (particle density, particle elasticity modulus) are applicable to any particle, regardless of their degree of irregularity. However, the test procedures used in the case of the interaction properties are not always valid when non-spherical particles are considered. This is especially noticeable in the test used for the determination of the particle-wall restitution coefficient and, to a lesser extent, in the one used for obtaining the particle-particle restitution coefficient. In this sense, it is necessary to establish modified or improved testing procedures applicable to non-regular particles or, alternatively, to establish alternative procedures (such as calibration procedures) to obtain a more reliable value.

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